

CRF Errors Edited by the STIC Systems Branch

Serial Number: 10/532,868

CRF Edit Date: 5/12/05
Edited by: AC

___ Realigned nucleic acid/amino acid numbers/text in cases where the sequence text "wrapped" to the next line

___ Corrected the SEQ ID NO. Sequence numbers edited were:

___ Inserted or corrected a nucleic number at the end of a nucleic line. SEQ ID NO's edited:

___ Deleted: / invalid beginning/end-of-file text ; ___ page numbers

___ Inserted mandatory headings/numeric identifiers, specifically:

___ Moved responses to same line as heading/numeric identifier, specifically:

___ Other:



PCT

RAW SEQUENCE LISTING

DATE: 05/12/2005

PATENT APPLICATION: US/10/532,868

TIME: 17:12:14

Input Set : A:\PTO.AMC.txt

Output Set: N:\CRF4\05122005\J532868.raw

3 <110> APPLICANT: Commissariat a l Etude Atomique (CEA)
 4 Centre National de la Recherche Scientifique (CNRS)
 6 <120> TITLE OF INVENTION: A method for performing restrained dynamics docking of one
 or
 7 multiple substrates on multi-specific enzymes
 9 <130> FILE REFERENCE: D20647
 C--> 11 <140> CURRENT APPLICATION NUMBER: US/10/532,868
 C--> 11 <141> CURRENT FILING DATE: 2005-04-28
 11 <150> PRIOR APPLICATION NUMBER: US 60/421,569
 12 <151> PRIOR FILING DATE: 2002-10-28
 14 <160> NUMBER OF SEQ ID NOS: 18
 16 <170> SOFTWARE: PatentIn version 3.2
 18 <210> SEQ ID NO: 1
 19 <211> LENGTH: 403
 20 <212> TYPE: PRT
 21 <213> ORGANISM: Fusarium oxysporum
 23 <220> FEATURE:
 24 <223> OTHER INFORMATION: P450 Nor, crystal structure from
 26 <400> SEQUENCE: 1
 28 Met Ala Ser Gly Ala Pro Ser Phe Pro Phe Ser Arg Ala Ser Gly Pro
 29 1 5 10 15
 31 Glu Pro Pro Ala Glu Phe Ala Lys Leu Arg Ala Thr Asn Pro Val Ser
 32 20 25 30
 34 Gln Val Lys Leu Phe Asp Gly Ser Leu Ala Trp Leu Val Thr Lys His
 35 35 40 45
 37 Lys Asp Val Cys Phe Val Ala Thr Ser Glu Lys Leu Ser Lys Val Arg
 38 50 55 60
 40 Thr Arg Gln Gly Phe Pro Glu Leu Ser Ala Ser Gly Lys Gln Ala Ala
 42 65 70 75 80
 44 Lys Ala Lys Pro Thr Phe Val Asp Met Asp Pro Pro Glu His Met His
 45 85 90 95
 47 Gln Arg Ser Met Val Glu Pro Thr Phe Thr Pro Glu Ala Val Lys Asn
 48 100 105 110
 50 Leu Gln Pro Tyr Ile Gln Arg Thr Val Asp Asp Leu Leu Glu Gln Met
 51 115 120 125
 53 Lys Gln Lys Gly Cys Ala Asn Gly Pro Val Asp Leu Val Lys Glu Phe
 54 130 135 140
 56 Ala Leu Pro Val Pro Ser Tyr Ile Ile Tyr Thr Leu Leu Gly Val Pro
 57 145 150 155 160
 59 Phe Asn Asp Leu Glu Tyr Leu Thr Gln Gln Asn Ala Ile Arg Thr Asn
 60 165 170 175
 62 Gly Ser Ser Thr Ala Arg Glu Ala Ser Ala Ala Asn Gln Glu Leu Leu
 63 180 185 190
 65 Asp Tyr Leu Ala Ile Leu Val Glu Gln Arg Leu Val Glu Pro Lys Asp

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Input Set : A:\PTO.AMC.txt

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66          195          200          205
68 Asp Ile Ile Ser Lys Leu Cys Thr Glu Gln Val Lys Pro Gly Asn Ile
69          210          215          220
71 Asp Lys Ser Asp Ala Val Gln Ile Ala Phe Leu Leu Val Ala Gly
72 225          230          235          240
74 Asn Ala Thr Met Val Asn Met Ile Ala Leu Gly Val Ala Thr Leu Ala
75          245          250          255
77 Gln His Pro Asp Gln Leu Ala Gln Leu Lys Ala Asn Pro Ser Leu Ala
78          260          265          270
80 Pro Gln Phe Val Glu Glu Leu Cys Arg Tyr His Thr Ala Ser Ala Leu
81          275          280          285
83 Ala Ile Lys Arg Thr Ala Lys Glu Asp Val Met Ile Gly Asp Lys Leu
84          290          295          300
86 Val Arg Ala Asn Glu Gly Ile Ile Ala Ser Asn Gln Ser Ala Asn Arg
87 305          310          315          320
89 Asp Glu Glu Val Phe Glu Asn Pro Asp Glu Phe Asn Met Asn Arg Lys
90          325          330          335
92 Trp Pro Pro Gln Asp Pro Leu Gly Phe Gly Phe Gly Asp His Arg Cys
93          340          345          350
95 Ile Ala Glu His Leu Ala Lys Ala Glu Leu Thr Thr Val Phe Ser Thr
96          355          360          365
98 Leu Tyr Gln Lys Phe Pro Asp Leu Lys Val Ala Val Pro Leu Gly Lys
99          370          375          380
101 Ile Asn Tyr Thr Pro Leu Asn Arg Asp Val Gly Ile Val Asp Leu Pro
102 385          390          395          400
104 Val Ile Phe
107 <210> SEQ ID NO: 2
108 <211> LENGTH: 403
109 <212> TYPE: PRT
110 <213> ORGANISM: Saccharopolyspora erythraea
112 <220> FEATURE:
113 <223> OTHER INFORMATION: P450 EryF, crystal structure 1oxa
115 <400> SEQUENCE: 2
117 Ala Thr Val Pro Asp Leu Glu Ser Asp Ser Phe His Val Asp Trp Tyr
118 1          5          10          15
120 Ser Thr Tyr Ala Glu Leu Arg Glu Thr Ala Pro Val Thr Pro Val Arg
121          20          25          30
123 Phe Leu Gly Gln Asp Ala Trp Leu Val Thr Gly Tyr Asp Glu Ala Lys
124          35          40          45
126 Ala Ala Leu Ser Asp Leu Arg Leu Ser Ser Asp Pro Lys Lys Lys Tyr
127          50          55          60
129 Pro Gly Val Glu Val Glu Phe Pro Ala Tyr Leu Gly Phe Pro Glu Asp
130 65          70          75          80
132 Val Arg Asn Tyr Phe Ala Thr Asn Met Gly Thr Ser Asp Pro Pro Thr
133          85          90          95
135 His Thr Arg Leu Arg Lys Leu Val Ser Gln Glu Phe Thr Val Arg Arg
136          100          105          110
138 Val Glu Ala Met Arg Pro Arg Val Glu Gln Ile Thr Ala Glu Leu Leu
139          115          120          125

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Input Set : A:\PTO.AMC.txt

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141 Asp Glu Val Gly Asp Ser Gly Val Val Asp Ile Val Asp Arg Phe Ala
142      130      135      140
144 His Pro Leu Pro Ile Lys Val Ile Cys Glu Leu Leu Gly Val Asp Glu
145 145      150      155      160
147 Ala Ala Arg Gly Ala Phe Gly Arg Trp Ser Ser Glu Ile Leu Val Met
148      165      170      175
150 Asp Pro Glu Arg Ala Glu Gln Arg Gly Gln Ala Ala Arg Glu Val Val
151      180      185      190
153 Asn Phe Ile Leu Asp Leu Val Glu Arg Arg Arg Thr Glu Pro Gly Asp
154      195      200      205
156 Asp Leu Leu Ser Ala Leu Ile Ser Val Gln Asp Asp Asp Asp Gly Arg
157      210      215      220
159 Leu Ser Ala Asp Glu Leu Thr Ser Ile Ala Leu Val Leu Leu Leu Ala
160 225      230      235      240
162 Gly Phe Glu Ala Ser Val Ser Leu Ile Gly Ile Gly Thr Tyr Leu Leu
163      245      250      255
165 Leu Thr His Pro Asp Gln Leu Ala Leu Val Arg Ala Asp Pro Ser Ala
166      260      265      270
168 Leu Pro Asn Ala Val Glu Glu Ile Leu Arg Tyr Ile Ala Pro Pro Glu
169      275      280      285
171 Thr Thr Thr Arg Phe Ala Ala Glu Glu Val Glu Ile Gly Gly Val Ala
172      290      295      300
174 Ile Pro Gln Tyr Ser Thr Val Leu Val Ala Asn Gly Ala Ala Asn Arg
175 305      310      315      320
177 Asp Pro Ser Gln Phe Pro Asp Pro His Arg Phe Asp Val Thr Arg Asp
178      325      330      335
180 Thr Arg Gly His Leu Ser Phe Gly Gln Gly Ile His Phe Cys Met Gly
181      340      345      350
183 Arg Pro Leu Ala Lys Leu Glu Gly Glu Val Ala Leu Arg Ala Leu Phe
184      355      360      365
186 Gly Arg Phe Pro Ala Leu Ser Leu Gly Ile Asp Ala Asp Asp Val Val
187      370      375      380
189 Trp Arg Arg Ser Leu Leu Leu Arg Gly Ile Asp His Leu Pro Val Arg
190 385      390      395      400
192 Leu Asp Gly
195 <210> SEQ ID NO: 3
196 <211> LENGTH: 412
197 <212> TYPE: PRT
198 <213> ORGANISM: Pseudomonas sp.
200 <220> FEATURE:
201 <223> OTHER INFORMATION: P450 Terp, crystal structure 1cpt
203 <400> SEQUENCE: 3
205 Met Asp Ala Arg Ala Thr Ile Pro Glu His Ile Ala Arg Thr Val Ile
206 1      5      10      15
208 Leu Pro Gln Gly Tyr Ala Asp Asp Glu Val Ile Tyr Pro Ala Phe Lys
209      20      25      30
211 Trp Leu Arg Asp Glu Gln Pro Leu Ala Met Ala His Ile Glu Gly Tyr
212      35      40      45
214 Asp Pro Met Trp Ile Ala Thr Lys His Ala Asp Val Met Gln Ile Gly

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```

215      50      55      60
217 Lys Gln Pro Gly Leu Phe Ser Asn Ala Glu Gly Ser Glu Ile Leu Tyr
218 65      70      75      80
220 Asp Gln Asn Asn Glu Ala Phe Met Arg Ser Ile Ser Gly Gly Cys Pro
221      85      90      95
223 His Val Ile Asp Ser Leu Thr Ser Met Asp Pro Pro Thr His Thr Ala
224      100      105      110
226 Tyr Arg Gly Leu Thr Leu Asn Trp Phe Gln Pro Ala Ser Ile Arg Lys
227      115      120      125
229 Leu Glu Glu Asn Ile Arg Arg Ile Ala Gln Ala Ser Val Gln Arg Leu
230      130      135      140
232 Leu Asp Phe Asp Gly Glu Cys Asp Phe Met Thr Asp Cys Ala Leu Tyr
233 145      150      155      160
235 Tyr Pro Leu His Val Val Met Thr Ala Leu Gly Val Pro Glu Asp Asp
236      165      170      175
238 Glu Pro Leu Met Leu Lys Leu Thr Gln Asp Phe Phe Gly Val Glu Ala
239      180      185      190
241 Ala Arg Arg Phe His Glu Thr Ile Ala Thr Phe Tyr Asp Tyr Phe Asn
242      195      200      205
244 Gly Phe Thr Val Asp Arg Arg Ser Cys Pro Lys Asp Asp Val Met Ser
245      210      215      220
247 Leu Leu Ala Asn Ser Lys Leu Asp Gly Asn Tyr Ile Asp Asp Lys Tyr
248 225      230      235      240
250 Ile Asn Ala Tyr Tyr Val Ala Ile Ala Thr Ala Gly His Asp Thr Thr
251      245      250      255
253 Ser Ser Ser Ser Gly Gly Ala Ile Ile Gly Leu Ser Arg Asn Pro Glu
254      260      265      270
256 Gln Leu Ala Leu Ala Lys Ser Asp Pro Ala Leu Ile Pro Arg Leu Val
257      275      280      285
259 Asp Glu Ala Val Arg Trp Thr Ala Pro Val Lys Ser Phe Met Arg Thr
260      290      295      300
262 Ala Leu Ala Asp Thr Glu Val Arg Gly Gln Asn Ile Lys Arg Gly Asp
263 305      310      315      320
265 Arg Ile Met Leu Ser Tyr Pro Ser Ala Asn Arg Asp Glu Glu Val Phe
266      325      330      335
268 Ser Asn Pro Asp Glu Phe Asp Ile Thr Arg Phe Pro Asn Arg His Leu
269      340      345      350
271 Gly Phe Gly Trp Gly Ala His Met Cys Leu Gly Gln His Leu Ala Lys
272      355      360      365
274 Leu Glu Met Lys Ile Phe Phe Glu Glu Leu Leu Pro Lys Leu Lys Ser
275      370      375      380
277 Val Glu Leu Ser Gly Pro Pro Arg Leu Val Ala Thr Asn Phe Val Gly
278 385      390      395      400
280 Gly Pro Lys Asn Val Pro Ile Arg Phe Thr Lys Ala
281      405      410
283 <210> SEQ ID NO: 4
284 <211> LENGTH: 414
285 <212> TYPE: PRT
286 <213> ORGANISM: Pseudomonas putida

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288 <220> FEATURE:

289 <223> OTHER INFORMATION: P450 Cam, crystal structure 3cpp

291 <400> SEQUENCE: 4

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293 Thr Thr Glu Thr Ile Gln Ser Asn Ala Asn Leu Ala Pro Leu Pro Pro
294 1          5          10          15
296 His Val Pro Glu His Leu Val Phe Asp Phe Asp Met Tyr Asn Pro Ser
297          20          25          30
299 Asn Leu Ser Ala Gly Val Gln Glu Ala Trp Ala Val Leu Gln Glu Ser
300          35          40          45
302 Asn Val Pro Asp Leu Val Trp Thr Arg Cys Asn Gly Gly His Trp Ile
303          50          55          60
305 Ala Thr Arg Gly Gln Leu Ile Arg Glu Ala Tyr Glu Asp Tyr Arg His
306 65          70          75          80
308 Phe Ser Ser Glu Cys Pro Phe Ile Pro Arg Glu Ala Gly Glu Ala Tyr
309          85          90          95
311 Asp Phe Ile Pro Thr Ser Met Asp Pro Pro Glu Gln Arg Gln Phe Arg
312          100         105         110
314 Ala Leu Ala Asn Gln Val Val Gly Met Pro Val Val Asp Lys Leu Glu
315          115         120         125
317 Asn Arg Ile Gln Glu Leu Ala Cys Ser Leu Ile Glu Ser Leu Arg Pro
318          130         135         140
320 Gln Gly Gln Cys Asn Phe Thr Glu Asp Tyr Ala Glu Pro Phe Pro Ile
321 145         150         155         160
323 Arg Ile Phe Met Leu Leu Ala Gly Leu Pro Glu Glu Asp Ile Pro His
324          165         170         175
326 Leu Lys Tyr Leu Thr Asp Gln Met Thr Arg Pro Asp Gly Ser Met Thr
327          180         185         190
329 Phe Ala Glu Ala Lys Glu Ala Leu Tyr Asp Tyr Leu Ile Pro Ile Ile
330          195         200         205
332 Glu Gln Arg Arg Gln Lys Pro Gly Thr Asp Ala Ile Ser Ile Val Ala
333          210         215         220
335 Asn Gly Gln Val Asn Gly Arg Pro Ile Thr Ser Asp Glu Ala Lys Arg
336 225         230         235         240
338 Met Cys Gly Leu Leu Leu Val Gly Gly Leu Asp Thr Val Val Asn Phe
339          245         250         255
341 Leu Ser Phe Ser Met Glu Phe Leu Ala Lys Ser Pro Glu His Arg Gln
342          260         265         270
344 Glu Leu Ile Glu Arg Pro Glu Arg Ile Pro Ala Ala Cys Glu Glu Leu
345          275         280         285
347 Leu Arg Arg Phe Ser Leu Val Ala Asp Gly Arg Ile Leu Thr Ser Asp
348          290         295         300
350 Tyr Glu Phe His Gly Val Gln Leu Lys Lys Gly Asp Gln Ile Leu Leu
351 305         310         315         320
353 Pro Gln Met Leu Ser Gly Leu Asp Glu Arg Glu Asn Ala Cys Pro Met
354          325         330         335
356 His Val Asp Phe Ser Arg Gln Lys Val Ser His Thr Thr Phe Gly His
357          340         345         350
359 Gly Ser His Leu Cys Leu Gly Gln His Leu Ala Arg Arg Glu Ile Ile
360          355         360         365

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VERIFICATION SUMMARY

PATENT APPLICATION: US/10/532,868

DATE: 05/12/2005

TIME: 17:12:15

Input Set : A:\PTO.AMC.txt

Output Set: N:\CRF4\05122005\J532868.raw

L:11 M:270 C: Current Application Number differs, Replaced Current Application No

L:11 M:271 C: Current Filing Date differs, Replaced Current Filing Date